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Self-consistent description of local density dynamics in simple liquids. the case of molten lithium

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Abstract

© 2018 IOP Publishing Ltd. The dynamic structure factor is the quantity, which can be measured by means of Brillouin light-scattering as well as by means of inelastic scattering of neutrons and x-rays. The spectral (or frequency) moments of the dynamic structure factor define directly the sum rules of the scattering law. The theoretical scheme formulated in this study allows one to describe the dynamics of local density fluctuations in simple liquids and to obtain the expression of the dynamic structure factor in terms of the spectral moments. The theory satisfies all the sum rules, and the obtained expression for the dynamic structure factor yields correct extrapolations into the hydrodynamic limit as well as into the free-particle dynamics limit. We discuss correspondence of this theory with the generalized hydrodynamics and with the viscoelastic models, which are commonly used to analyze the data of inelastic neutron and x-ray scattering in liquids. In particular, we reveal that the postulated condition of the viscoelastic model for the memory function can be directly obtained within the presented theory. The dynamic structure factor of liquid lithium is computed on the basis of the presented theory, and various features of the scattering spectra are evaluated. It is found that the theoretical results are in agreement with inelastic x-ray scattering data.

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Keywords

density fluctuations, liquid metals, liquids, microscopic dynamics

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